On the geometry of similarity search: dimensionality curse and concentration of measure[‡]

Vladimir Pestov*

School of Mathematical and Computing Sciences, Victoria University of Wellington, P.O. Box 600, Wellington, New Zealand.

Abstract

We suggest that the curse of dimensionality affecting the similarity-based search in large datasets is a manifestation of the phenomenon of concentration of measure on high-dimensional structures. We prove that, under certain geometric assumptions on the query domain Ω and the dataset X, if Ω satisfies the so-called concentration property, then for most query points x^* the ball of radius $(1 + \epsilon)d_X(x^*)$ centred at x^* contains either all points of X or else at least $C_1 \exp(-C_2\epsilon^2 n)$ of them. Here $d_X(x^*)$ is the distance from x^* to the nearest neighbour in X and n is the dimension of Ω .

Keywords

Data structures, databases, information retrieval, computational geometry, performance evaluation

1. Introduction

As the size of datasets in existence grows at an amazing rate (see e.g. Section 4.1 in [11]) and workloads become ever more sophisticated, algorithms for similarity-based data retrieval often slow down exponentially with dimension, sometimes reducing to an exhaustive search ('the curse of dimensionality') [2, 3, 1, 14]. It is important to try and understand the common geometric nature of the dimensionality curse for a great variety of different, often non-euclidean, metric spaces representing data structures [4, 5, 6, 13].

In this Letter we suggest that the curse of dimensionality is a manifestation of the phenomenon of concentration of measure on high-dimensional structures.

This phenomenon is an important discovery of modern analysis, observed in a wide range of situations [7, 9, 10, 12]. Roughly speaking, a set Ω equipped with a distance and a probability measure has the concentration property if already for small values of $\epsilon > 0$ the ' ϵ -fattening' of every subset containing at least 1/2 of all elements of Ω contains all points of Ω apart from a set of almost vanishing measure $\alpha(\epsilon)$. Here α is the so-called concentration function of Ω . Many 'naturally occurring' high-dimensional structures possess the concentration property: the n-dimensional

[‡]Partially supported by the Marsden Fund grant VUW703 of the Royal Society of New Zealand.

^{*}E-mail: vova@@mcs.vuw.ac.nz

URL: http://www.vuw.ac.nz/~vova

Preprint data: RP-99-01, School of Mathematical and Computing Sciences, Victoria University of Wellinton, January 1999.

sphere \mathbb{S}^n , Euclidean unit ball \mathbb{B}^n , Hamming cube $\{0,1\}^n$, groups of permutations S_n all have concentration functions of the form $\alpha(\epsilon) = O(1) \exp(-O(1)\epsilon^2 n)$.

Here we will address just one aspect of 'dimensionality curse,' informally described in [3] as follows:

'It seems ... that this [exponential] complexity might be inherent in any algorithm for solving closest point problems because a point in a high-dimensional space can have many "close" neighbours.'

To formalise this account, we borrow a concept from [2]. A similarity query is called ϵ -unstable for an $\epsilon > 0$ if most points if the dataset X are at a distance $< (1+\epsilon)d_X(x^*)$ from the query point x^* , where d_X denotes the distance to the nearest neighbour in the dataset X. Query instability was shown in [2] to occur under some probability assumptions on the query distribution, and it was argued that asking unstable queries is partly responsible for the dimensionality curse. It seems to us that even more important is a 'local' version of query instability, where the number of data points located at a distance $< (1 + \epsilon)d_X(x^*)$ from a query point x^* grows exponentially in the dimension of the query domain. If such an effect prevails in a given workload, then answering the range query of radius $(1 + \epsilon)d_X(x^*)$ obviously takes an average expected exponential time, even though the query may be globally stable.

In our model, a dataset X is a finite metric subspace of a metric space Ω of query points, the latter being equipped with a probability measure reflecting the query distribution. We assume that Ω has the concentration property in the sense that $\alpha(\epsilon) = O(1) \exp(-O(1)\epsilon^2 n)$, where n is the 'dimension' of the query domain Ω . Our assumption on the way X sits in Ω is of a homogeneity type: the radii of open balls centred at x and having measure 1/2 are (almost) the same for all datapoints x.

Under such assumptions we prove that if $\epsilon > 0$, then for all query points $x^* \in \Omega$, apart from a set of measure $O(1) \exp(-O(1)\epsilon^2 n)$, the open ball of radius $(1+\epsilon)d_X(x^*)$ centred at x^* contains either all points of the dataset X or else at least $C_1 \exp(C_2\epsilon^2 n)$ of them for some $C_1, C_2 > 0$. Thus, a typical range query of radius $(1+\epsilon)d_X(x^*)$ is either unstable or takes an exponential time to answer. In particular, most queries are unstable if the size of X grows subexponentially in n.

In Conclusion we explain a possible constructive significance of our results.

2. Similarity workloads

Our model builds on the approaches of [5, 6] and [8]. A similarity workload is a quadruple (Ω, d, μ, X) , where

- 1. Ω is a (possibly infinite) set called the *domain*, whose elements are *query points*.
- 2. d is a metric on Ω , the dissimilarity measure.
- 3. μ is a Borel probability measure on the metric space (Ω, d) , reflecting the query point distribution.
- 4. X is a finite subset of Ω , called the *instance*, or the *dataset* proper, whose elements are *data points*.

Recall that a triple (Ω, d, μ) formed by a metric space (Ω, d) and a probability Borel measure μ on it is called a *probability metric space*. Thus, a similarity workload is a probability metric space Ω together with a distinguished finite metric subspace X.

Similarity queries are of two major types: a range query centred at $x^* \in \Omega$ of radius $\epsilon > 0$ (the set of all $x \in X$ with $d(x, x^*) < \epsilon$), and a k-nearest neighbours (k-NN) query centred at $x^* \in \Omega$, where $k \in \mathbb{N}$.

Following [2], we say that a similarity query centred at x^* is ϵ -unstable for an $\epsilon > 0$ if

$$|\{x \in X : d(x^*, x) \le (1 + \epsilon)d_X(x^*)\}| > \frac{|X|}{2},$$

where $d_X(x^*) = \min\{d(x^*, x) : x \in X\}$ is the distance from x^* to the nearest neighbour in X. In [2] the following new type of queries is proposed.

• An ϵ -radius nearest neighbours query centred at a point $x^* \in \Omega$, where $\epsilon > 0$, is a range query centred at x^* of the radius $(1 + \epsilon)d_X(x^*)$.

3. The concentration phenomenon

The concentration function, $\alpha = \alpha_{\Omega}$, of a probability metric space Ω is defined for each $\epsilon > 0$ by

$$\alpha_{\Omega}(\epsilon) = 1 - \inf \left\{ \mu\left(\mathcal{O}_{\epsilon}(A)\right) : A \subseteq \Omega \text{ is Borel and } \mu(A) \ge \frac{1}{2} \right\}$$
 (3.1)

and $\alpha_{\Omega}(0) = 1/2$. It is a decreasing function in ϵ .

A family $(\Omega_n)_{n=1}^{\infty}$ of probability metric spaces is called a $L\acute{e}vy$ family if for each $\epsilon > 0$, $\alpha_{\Omega_n}(\epsilon) \to 0$ as $n \to \infty$, and a normal $L\acute{e}vy$ family (with constants $C_1, C_2 > 0$) if for all n and $\epsilon > 0$

$$\alpha_{\Omega_n}(\epsilon) \le C_1 e^{-C_2 \epsilon^2 n}$$

All the families listed below are normal Lévy families, see [7, 9, 10] for exact values of constants and further examples.

Examples 3.1. (1) The *n*-dimensional unit spheres \mathbb{S}^n equipped with the (unique) rotation-invariant probability measure and the geodesic distance. (2) The same, with the Euclidean distance. (3) The Hamming cubes $\{0,1\}^n$ of all binary strings of length n, equipped with the normalised Hamming distance $d(s,t) = \frac{1}{n} |\{i : s_i \neq t_i\}|$ and the normalised counting measure $\mu_{\sharp}(A) = |A|/|X|$. (4) The groups SO(n) of $n \times n$ orthogonal matrices with determinant 1, equipped with the geodesic distance and the Haar measure. (5) The Euclidean balls \mathbb{B}^n with the n-volume and Euclidean distance. (6) The tori \mathbb{T}^n with the normalised geodesic distance and product measure. (7) The hypercubes $[0,1]^n$ with the normalised Euclidean (or l_1) distance.

More Lévy families can be obtained using operations described in [7], Sect. 2. Let $f: \Omega \to \mathbb{R}$ be a Lipschitz-1 function:

$$\forall x, y \in \Omega, |f(x) - f(y)| \le d(x, y).$$

Denote by M a median (or Lévy mean) of f, that is, a real number with

$$\mu(\{x \in X : f(x) \le M\}) = \mu(\{x \in X : f(x) \ge M\}).$$

Proposition 3.2. For every
$$\epsilon > 0$$
, $\mu\left(f^{-1}(M - \epsilon, M + \epsilon)\right) \ge 1 - 2\alpha(\epsilon)$.

The phenomenon of concentration of measure on high-dimensional structures refers to the above situation, in which the function f 'concentrates near one value.' See [7, 9, 10, 12].

4. Concentration and similarity workloads

Let Ω be a probability metric space with the concentration function $\alpha = \alpha_{\Omega}$. The following is quite immediate.

Lemma 4.1. Let
$$A \subseteq \Omega$$
, $\delta > 0$, and $\mu(A) > \alpha(\delta)$. Then $\mu(\mathcal{O}_{\delta}(A)) > 1/2$.

Lemma 4.2. Let $\delta > 0$, and let γ be a collection of subsets $A \subseteq \Omega$ of measure $\mu(A) \leq \alpha(\delta)$ each, satisfying $\mu(\cup \gamma) \geq 1/2$. Then the 2δ -neighbourhood of every point $x \in \Omega$, apart from a set of measure at most $\frac{1}{2}\alpha(\delta)^{\frac{1}{2}}$, meets at least $\lceil \frac{1}{2}\alpha(\delta)^{-\frac{1}{2}} \rceil$ elements of γ .

Proof. Partition γ into a collection of pairwise disjoint subfamilies γ_i , $i \in I$ in such a way that for every i, $\alpha(\delta) \leq \mu(A_i) < 2\alpha(\delta)$, where $A_i = \cup \gamma_i$. Clearly, $(1/4)\alpha(\delta)^{-1} \leq |I| \leq (1/2)\alpha(\delta)^{-1}$. Select a subset $J \subseteq I$ with $|J| = \lceil \frac{1}{2}\alpha(\delta)^{-\frac{1}{2}} \rceil$. Lemma 4.1 implies that

$$\mu\left(\mathcal{O}_{2\delta}(A_i)\right) \ge \mu\left(\mathcal{O}_{\delta}\left(\mathcal{O}_{\delta}A_i\right)\right) \ge 1 - \alpha(\delta),$$

and therefore $\cap_{i\in J}(\mathcal{O}_{2\delta}(A_i))$ has measure at most $1-|J|\alpha(\delta)$.

Let (Ω, d, μ, X) be a similarity workload, with α as above. Denote by M a median value of the function d_X (distance to X) on Ω .

Lemma 4.3. Let $\delta > 0$. Then for all points $x^* \in \Omega$, except for a set of total mass at most $2\alpha(\delta)$, the distance to the nearest neighbour in X is in the interval $(M-\delta, M+\delta)$.

Proof. The function $x^* \to d_X(x^*)$ is Lipschitz-1 on Ω , and Prop. 3.2 applies.

Definition 4.4. Let (Ω, d, μ, X) be a similarity workload. For an $x \in X$, denote by R_x the maximal radius of an open ball in Ω centred at x of measure $\leq 1/2$. Let $\epsilon > 0$. We say that X is weakly ϵ -homogeneous in Ω if all radii R_x , $x \in X$ belong to an interval of length $< \epsilon$.

Examples 4.5. (1) X is weakly ϵ -homogeneous for every $\epsilon > 0$ if the group of motions preserving the measure acts transitively on Ω . Such are spaces 1-4, 6 in Example 3.1. (2) A subspace X of the ball \mathbb{B}^n is weakly ϵ -homogeneous if X is contained in a spherical shell of thickness ϵ . (3) If we independently throw in Ω N points x_1, x_2, \ldots, x_N , distributed with respect to the measure μ , then one can show that, with probability $\geq 1 - 2N\alpha(\epsilon/2)$, the dataset $X = \{x_1, \ldots, x_N\}$ is weakly ϵ -homogeneous.

5. Query instability: local and global

Theorem 5.1. Let (Ω, d, μ, X) be a similarity workload. Denote by M a median value of the distance from a query point in Ω to its nearest neighbour in X. Let $0 < \epsilon < 1$, and assume that the instance X is weakly $(M\epsilon/6)$ -homogeneous in Ω .

Then for all points $x^* \in \Omega$, apart from a set of total mass at most $3\alpha(M\epsilon/6)$, the open ball of radius $(1+\epsilon)d_X(x^*)$ centred at x^* contains at least

$$\min\left\{|X|, \left\lceil \frac{1}{2\alpha(M\epsilon/6)^{\frac{1}{2}}} \right\rceil\right\} \tag{5.1}$$

Proof. Denote by R the minimum of the radii $R_x, x \in X$. Let $\Delta = R - M$.

- (1) If $\Delta > M\epsilon/6$, then by Lemma 4.1 the measure of the ball $\mathcal{O}_M(x)$ cannot exceed $\alpha(\Delta) \leq \alpha(M\epsilon/6)$, for otherwise the measure of $\mathcal{O}_R(x)$ would be > 1/2. In particular, $|X| \geq \frac{1}{2}\alpha(M\epsilon/6)^{-1}$. According to Lemma 4.2 applied to the balls $\mathcal{O}_M(x)$, $x \in X$ with $\delta = M\epsilon/6$, for all $x^* \in \Omega$ apart from a set of measure $\leq \frac{1}{2}\alpha(M\epsilon/6)^{\frac{1}{2}}$, the $(M\epsilon/3)$ -neighbourhood of x^* meets at least $\lceil \frac{1}{2}\alpha(M\epsilon/6)^{-\frac{1}{2}} \rceil$ of such balls.
- (2) If $\Delta \leq M\epsilon/6$ (in particular, if $|X| < \frac{1}{2}\alpha(M\epsilon/6)^{-\frac{1}{2}} \leq \frac{1}{2}\alpha(M\epsilon/6)^{-1}$, cf. the previous paragraph), then $R_x + M\epsilon/6 \leq M(1+\epsilon/2)$. Denote by X' a subset of X of cardinality $\min\{|X|, \frac{1}{2}\alpha(M\epsilon/6)^{-\frac{1}{2}}\}$. Since the measure of every ball $\mathcal{O}_{M(1+\epsilon/2)}(x)$ is at least $1 \alpha(M\epsilon/6)$, for all $x^* \in \Omega$ apart from a set of measure $\leq \frac{1}{2}\alpha(M\epsilon/6)^{\frac{1}{2}}$, the $(M\epsilon/2)$ -neighbourhood of x^* meets every ball $\mathcal{O}_M(x)$, $x \in X'$.

As a consequence of Lemma 4.3 with $\delta = M\epsilon/4$, for all $x^* \in \Omega$ apart from a set of measure at most $2\alpha(M\epsilon/4)$, one has $|d_X(x^*)-M| < M\epsilon/4$ and therefore $M(1+\epsilon/2) \le d_X(x^*)(1+\epsilon)$. It remains to notice that $\frac{1}{2}\alpha(M\epsilon/6)^{\frac{1}{2}} + 2\alpha(M\epsilon/4) \le 3\alpha(M\epsilon/6)^{\frac{1}{2}}$. \square

Asymptotic results. Let $(\Omega_n, d_n, \mu_n, X_n)$ be an infinite collection of workloads. Denote by M_n the median distances from points of Ω_n to their nearest neighbours in X_n . We make the following standing assumptions.

- (1) The query domains (Ω_n, d_n, μ_n) form a normal Lévy family.
- (2) The values M_n are bounded away from zero: $M_n \ge M > 0$ for all $n \in \mathbb{N}$.

Remark 5.2. The latter condition is only violated in very densely populated domains. For example, if $\Omega_n = \mathbb{S}^n$, then (2) is satisfied whenever the size of X_n is not superexponential in n. For Ω_n finite (2) is satisfied if $|X_n| \leq \alpha_{\Omega_n}(M) \cdot |\Omega_n|$.

Now let $0 < \epsilon < 1$.

(3) All the instances X_n are weakly $(M_n \epsilon/6)$ -homogeneous in Ω_n .

Corollary 5.3. Under the assumptions (1)-(3), for all query points $x^* \in \Omega_n$, apart from a set of measure $O(1) \exp(-O(1)M^2\epsilon^2 n)$, the open ball of radius $(1+\epsilon)d_X(x^*)$ centred at x^* contains either all elements of X or else at least $C_1 \exp(C_2M^2\epsilon^2 n)$ of them for some constants $C_1, C_2 > 0$ depending only on the family $(\Omega_n)_{n=1}^{\infty}$.

Corollary 5.4. Under the assumptions (1)-(3), for all query points x^* , apart from a set of measure $O(1) \exp(-O(1)M^2\epsilon^2 n)$, the ϵ -radius nearest neighbours query centred at x^* either is unstable or takes an exponential time (in n) to answer.

Corollary 5.5. In addition to (1)-(3), let the size of X_n grow subexponentially in n. Then for all query points $x^* \in \Omega_n$, apart from a set of measure $O(1) \exp(-O(1)M^2\epsilon^2 n)$, the similarity query centred at x^* is ϵ -unstable: all points of X_n are at a distance $< (1 + \epsilon)d_X(x^*)$ from x^* .

Example 5.6. It is easy to construct sequences of workloads in which most of similarity queries are 1-stable and yet for every $\epsilon > 0$ most of the ϵ -radius NN queries take time $C_1 \exp(C_2 \epsilon^2 n)$ to answer.

Let $\delta > 0$ be arbitrary. In a probability metric space Ω choose a maximal subset X with the property that every two different elements of X are at a distance $> \delta$ from

each other. It is easy to see that centres of all 1-unstable similarity queries in the workload (Ω, X) are contained in some ball of radius 4δ . Applying this procedure to every member of a normal Lévy family of homogeneous spaces of constant diameter D (a typical situation) and choosing $\delta < D/8$, we obtain a desired sequence of workloads, because one can then prove that $\liminf M_n \geq \delta/2$.

6. Conclusion

Our model links the 'curse of dimensionality' in multidimensional datasets to the phenomenon of concentration of measure on high-dimensional structures. All our assumptions on the query domain Ω and the dataset X are purely geometric. Our estimates are by no means optimal, as we just aimed at deriving exponential lower bounds in a wide variety of situations. We believe that the most general case (absence of homogeneity in any form) can be included in the picture as well and will address the issue in the future work. Other important directions for research are to apply the concentration phenomenon to indexability theory [8] and to performance analysis of concrete hierarchical tree index structures [3, 4, 5, 6, 13].

A possible constructive significance of our results is as follows. In practice, geometrically optimal dissimilarity measures are being routinely replaced with less precise distances that are computationally cheaper, with a view of subsequently discarding false hits. Such distances would in general lead to sharper concentration effects on the same measure space. It is therefore conceivable that using computationally more expensive distances will result in an overall speed-up.

ACKNOWLEDGEMENTS

I am grateful to Paolo Ciaccia for introducing me to the problematics of similarity-based information storage and retrieval, as well as for his hospitality and stimulating discussions during my visit to the University of Bologna in June 1998.

References

- [1] S. Berchtold, C. Böhm, D.A. Keim, and H.-P. Kriegl, A cost model for nearest neighbour search in high-dimensional data space, PODS'97 (Tucson, AZ), 78–86.
- [2] K. Beyer, J. Goldstein, R. Ramakrishnan, and U. Shaft, When is "nearest neighbor" meaning-ful?, Technical paper no. 226, CS dept., Univ. Wisconsin-Madison, to appear in: ICDT-99.
- [3] J.L. Bentley, B.W. Weide, and A.C. Yao, Optimal expected-time algorithms for closest point problems, ACM Trans. Math. Software 6 (1980), 563–580.
- [4] S. Brin, Near neighbor search in large metric spaces, in: Proc. of the 21st VLDB International Conf., Zurich, Switzerland, Sept. 1995, pp. 574–584.
- [5] P. Ciaccia, M. Patella, F. Rabitti, and P. Zezula, Performance of M-tree, an access method for similarity search in metric spaces, EC ESPRIT report, 24 February 1997, 25 pp., downloadable from http://www.ced.tuc.gr/hermes
- [6] P. Ciaccia, M. Patella, and P. Zezula, A cost model for similarity queries in metric spaces, in: Proc. 17-th Annual ACM Symposium on Principles of Database Systems (PODS'98), Seattle, WA, June 1998, pp. 59–68.
- [7] M. Gromov and V.D. Milman, A topological application of the isoperimetric inequality, Amer. J. Math. 105 (1983), 843–854.
- [8] J.M. Hellerstein, E. Koutsoupias, and C.H. Papadimitriou, On the analysis of indexing schemes, in: PODS'97, Tucson, AZ, pp. 249–256.
- [9] V.D. Milman, The heritage of P.Lévy in geometric functional analysis, Astérisque 157-158 (1988), 273-301.

- [10] V.D. Milman and G. Schechtman, Asymptotic Theory of Finite Dimensional Normed Spaces, Lecture Notes in Math. 1200, Springer-Verlag, 1986.
- [11] A. Silberschatz, M. Stonebraker, and J. Ullman (eds.), *Database research: achievements and opportunities into the 21st century*, Report of an NSF Workshop on the Future of Database Systems Research, May 26–27, 1995.
- [12] M. Talagrand, Concentration of measure and isoperimetric inequalities in product spaces, Publ. Math. IHES 81 (1995), 73–205.
- [13] J.K. Uhlmann, Satisfying general proximity/similarity queries with metric trees, Information Processing Lett. 40 (1991), 175–179.
- [14] R. Weber, H.-J. Schek, and S. Blott, A quantatitive analysis and performance study for similarity-search methods in high-dimensional spaces, in: Proceedings of the 24-th VLDB Conference, New York, 1998, pp. 194–205.